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Dynamical Difference Equations

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Abstract—Dynamical difference equations are motivated and developed. Conservation and covariance laws are proved. Illustrative examples are described and discussed. Newtonian equations are stressed, but extensions to relativity and quantum mechanics are indicated. The physical problem of convergence to the limit as the time step goes to zero is shown to reveal an area in which quantum mechanics and relativity are in disagreement. © 1998 Elsevier Science Ltd. All rights reserved.

Keywords—Physical experimentation, Discontinuous time, Particle modelling.

1. INTRODUCTION

Our purpose in this paper is to develop a dynamical approach to modelling the most fundamental activity in science, that is, experimentation.

Most importantly, in every experiment there is a clock and the clock will be included in our considerations. For this purpose, we let Δt be a positive number which represents the time between successive ticks of the clock and let the discrete times t_n be defined by $t_n = n\Delta t$, $n = 0, 1, 2, \dots$. Of necessity, any dynamical equation to be developed must depend on Δt and, therefore, will be a dynamical *difference* equation. Rates of change will be represented by forward difference quotients, and function values will be determined using arithmetic means.

We will concentrate primarily on Newtonian type difference equations for N-body problems. The three-body problem will be stressed, since all results for it extend directly to the general case. Throughout, *cgs* units are employed.

2. POTENTIALS AND FORCE FORMULAS

At time t_n and for $i = 1, 2, \dots, N$, let particle P_i of mass m_i be at $\vec{r}_{i,n} = (x_{i,n}, y_{i,n}, z_{i,n})$. Let the positive Euclidean distance between P_i and P_j, $i \neq j$, and at time t_n be $r_{ij,n} = r_{ji,n}$. The assumption that $r_{ij,n} > 0$ for $i \neq j$ implies conservation of mass. Let $\phi = \phi_{ij,n} = \phi(r_{ij,n})$, given in ergs, be a potential for the pair P_i and P_j, $i \neq j$. Then, the force $\vec{F}_{ij,n}$ on P_i due to P_j is defined by

$$\vec{F}_{ij,n} = -\frac{\phi(r_{ij,n+1}) - \phi(r_{ij,n})}{r_{ij,n+1} - r_{ij,n}} \, \frac{(1/2)(\vec{r}_{i,n+1} + \vec{r}_{i,n}) - (1/2)(\vec{r}_{j,n+1} + \vec{r}_{j,n})}{(1/2)(r_{ij,n+1} + r_{ij,n})}, \tag{2.1}$$

or, more simply, by

$$\vec{F}_{ij,n} = -\frac{\phi(r_{ij,n+1}) - \phi(r_{ij,n})}{r_{ij,n+1} - r_{ij,n}} \cdot \frac{(\vec{r}_{i,n+1} + \vec{r}_{i,n}) - (\vec{r}_{j,n+1} + \vec{r}_{j,n})}{(r_{ij,n+1} + r_{ij,n})}. \tag{2.2}$$

Since for most Newtonian potentials of interest [1–3], the singularity $r_{ij,n+1} = r_{ij,n}$ in (2.2) is removable, we proceed under the assumption that $r_{ij,n+1} \neq r_{ij,n}$.

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Note also, that

$$\vec{F}_{ij,n} = -\vec{F}_{ji,n},$$

which is called the law of action-reaction.

3. DYNAMICAL DIFFERENCE EQUATIONS

The three-body problem is now defined as follows. Given the initial positions and velocities of P_1, P_2, P_3, determine their motions if the system's dynamical equations are the difference equations

$$\frac{\vec{r}_{i,n+1} - \vec{r}_{i,n}}{\Delta t} = \frac{\vec{v}_{i,n+1} + \vec{v}_{i,n}}{2}, \tag{3.1}$$

$$\begin{aligned} m_i \frac{\vec{v}_{i,n+1} - \vec{v}_{i,n}}{\Delta t} = &-\frac{\phi(r_{ij,n+1}) - \phi(r_{ij,n})}{r_{ij,n+1} - r_{ij,n}} \cdot \frac{\vec{r}_{i,n+1} + \vec{r}_{i,n} - \vec{r}_{j,n+1} - \vec{r}_{j,n}}{r_{ij,n+1} + r_{ij,n}} \\ &- \frac{\phi(r_{ik,n+1}) - \phi(r_{ik,n})}{r_{ik,n+1} - r_{ik,n}} \cdot \frac{\vec{r}_{i,n+1} + \vec{r}_{i,n} - \vec{r}_{k,n+1} - \vec{r}_{k,n}}{r_{ik,n+1} + r_{ik,n}}, \end{aligned} \tag{3.2}$$

where $i = 1$ implies $j = 2$, $k = 3$; $i = 2$ implies $j = 1$, $k = 3$; $i = 3$ implies $j = 1$, $k = 2$.

For the general N-body problem, the right side of (3.2) need only be expanded so as to include the $N - 1$ force components each contributed by a particle different from P_i.

System (3.1),(3.2) constitutes 18 implicit recursion equations for the unknowns $x_{i,n+1}$, $y_{i,n+1}$, $z_{i,n+1}$, $v_{i,x,n+1}$, $v_{i,y,n+1}$, $v_{i,z,n+1}$ in the 18 knowns $x_{i,n}$, $y_{i,n}$, $z_{i,n}$, $v_{i,x,n}$, $v_{i,y,n}$, $v_{i,z,n}$, $i = 1, 2, 3$. As will be indicated by examples later, these equations are readily solvable by Newton's method [2].

4. CONSERVATION LAWS

We now prove fundamental conservation laws, that is, results which establish system invariants. This will be done for the three-body problem in a fashion which extends directly to the general case. Since we will concentrate only on the three-body problem, we allow N in this section to be a general index of summation. In addition, we assume the usual definition of kinetic energy.

THEOREM 4.1. *Independently of Δt, formulae (3.1),(3.2) are energy conserving, that is,*

$$K_N + \phi_N = K_0 + \phi_0, \qquad N = 1, 2, \dots .$$

PROOF. Define

$$W_N = \sum_{n=0}^{N-1} \sum_{i=1}^{3} m_i (\vec{r}_{i,n+1} - \vec{r}_{i,n}) \cdot \frac{(\vec{v}_{i,n+1} - \vec{v}_{i,n})}{\Delta t}. \tag{4.1}$$

With the aid of (3.1), then,

$$\begin{aligned} W_N &= \sum_{n=0}^{N-1} \sum_{i=1}^{3} m_i \frac{(\vec{r}_{i,n+1} - \vec{r}_{i,n})}{\Delta t} \cdot (\vec{v}_{i,n+1} - \vec{v}_{i,n}) \\ &= \sum_{n=0}^{N-1} \sum_{i=1}^{3} m_i \left(\frac{v_{i,n+1}^2}{2} - \frac{v_{i,n}^2}{2} \right) \\ &= \sum_{i=1}^{3} m_i \left[\left(\frac{v_{i,1}^2}{2} - \frac{v_{i,0}^2}{2} \right) + \left(\frac{v_{i,2}^2}{2} - \frac{v_{i,1}^2}{2} \right) + \left(\frac{v_{i,3}^2}{2} - \frac{v_{i,2}^2}{2} \right) + \cdots + \left(\frac{v_{i,N}^2}{2} - \frac{v_{i,N-1}^2}{2} \right) \right] \\ &= \frac{1}{2} m_1 v_{1,N}^2 + \frac{1}{2} m_2 v_{2,N}^2 + \frac{1}{2} m_3 v_{3,N}^2 - \frac{1}{2} m_1 v_{1,0}^2 - \frac{1}{2} m_2 v_{2,0}^2 - \frac{1}{2} m_3 v_{3,0}^2, \end{aligned}$$

so that

$$W_N = K_N - K_0.$$

Next, with the aid of (3.2) and the observation that $\vec{r}_i - \vec{r}_j = \vec{r}_{ji}$, one finds

$$\begin{aligned}
W_N = \sum_{n=0}^{N-1} \Bigg[& (\vec{r}_{1,n+1} - \vec{r}_{1,n}) \cdot \left\{ -\frac{\phi(r_{12,n+1}) - \phi(r_{12,n})}{r_{12,n+1} - r_{12,n}} \frac{\vec{r}_{1,n+1} + \vec{r}_{1,n} - \vec{r}_{2,n+1} - \vec{r}_{2,n}}{r_{12,n+1} + r_{12,n}} \right. \\
& \left. - \frac{\phi(r_{13,n+1}) - \phi(r_{13,n})}{r_{13,n+1} - r_{13,n}} \frac{\vec{r}_{1,n+1} + \vec{r}_{1,n} - \vec{r}_{3,n+1} - \vec{r}_{3,n}}{r_{13,n+1} + r_{13,n}} \right\} \\
& + (\vec{r}_{2,n+1} - \vec{r}_{2,n}) \cdot \left\{ -\frac{\phi(r_{12,n+1}) - \phi(r_{12,n})}{r_{12,n+1} - r_{12,n}} \frac{\vec{r}_{2,n+1} + \vec{r}_{2,n} - \vec{r}_{1,n+1} - \vec{r}_{1,n}}{r_{12,n+1} + r_{12,n}} \right. \\
& \left. - \frac{\phi(r_{23,n+1}) - \phi(r_{23,n})}{r_{23,n+1} - r_{23,n}} \frac{\vec{r}_{2,n+1} + \vec{r}_{2,n} - \vec{r}_{3,n+1} - \vec{r}_{3,n}}{r_{23,n+1} + r_{23,n}} \right\} \\
& + (\vec{r}_{3,n+1} - \vec{r}_{3,n}) \cdot \left\{ -\frac{\phi(r_{13,n+1}) - \phi(r_{13,n})}{r_{13,n+1} - r_{13,n}} \frac{\vec{r}_{3,n+1} + \vec{r}_{3,n} - \vec{r}_{1,n+1} - \vec{r}_{1,n}}{r_{13,n+1} + r_{13,n}} \right. \\
& \left. - \frac{\phi(r_{23,n+1}) - \phi(r_{23,n})}{r_{23,n+1} - r_{23,n}} \frac{\vec{r}_{3,n+1} + \vec{r}_{3,n} - \vec{r}_{2,n+1} - \vec{r}_{2,n}}{r_{23,n+1} + r_{23,n}} \right\} \\
= & \sum_{n=0}^{N-1} \left(-\phi_{12,n+1} - \phi_{13,n+1} - \phi_{23,n+1} + \phi_{12,n} + \phi_{13,n} + \phi_{23,n} \right) \\
= & -\phi_{12,N} - \phi_{13,N} - \phi_{23,N} + \phi_{12,0} + \phi_{13.0} + \phi_{23,0}.
\end{aligned}$$

Thus,

$$W_N = -\phi_N + \phi_0.$$

Hence,

$$\begin{aligned}
K_N - K_0 &= -\phi_N + \phi_0, \\
\Rightarrow K_N + \phi_N &= K_0 + \phi_0, \qquad N = 0, 1, 2, \dots .
\end{aligned}$$

∎

We turn then to linear momentum. The linear momentum $\vec{M}_i(t_n)$ of P_i at t_n is defined to be the vector

$$\vec{M}_{i,n} = m_i(v_{i,x,n}, v_{i,y,n}, v_{i,z,n}).$$

The linear momentum $\vec{M}_n$ of the three-body system at time t_n is defined to be

$$\vec{M}_n = \sum_{i=1}^{3} \vec{M}_{i,n}.$$

THEOREM 4.2. *Independently of Δt, the numerical method conserves linear momentum, that is,*

$$\vec{M}_N = \vec{M}_0, \qquad N = 0, 1, 2, \dots .$$

PROOF. From (3.2),

$$m_1 \left(v_{1,x,n+1} - v_{1,x,n}\right) + m_2 \left(v_{2,x,n+1} - v_{2,x,n}\right) + m_3 \left(v_{3,x,n+1} - v_{3,x,n}\right) = 0. \tag{4.2}$$

Summing both sides of (4.2) from $n = 0$ to $N - 1$ implies

$$m_1 v_{1,x,N} + m_2 v_{2,x,N} + m_3 v_{3,x,N} = C_1, \qquad N \geq 1,$$

in which

$$m_1 v_{1,x,0} + m_2 v_{2,x,0} + m_3 v_{3,x,0} = C_1.$$

Similarly,

$$m_1 v_{1,y,N} + m_2 v_{2,y,N} + m_3 v_{3,y,N} = C_2,$$
$$m_1 v_{1,z,N} + m_2 v_{2,z,N} + m_3 v_{3,z,N} = C_3,$$

in which

$$m_1 v_{1,y,0} + m_2 v_{2,y,0} + m_3 v_{3,y,0} = C_2,$$
$$m_1 v_{1,z,0} + m_2 v_{2,z,0} + m_3 v_{3,z,0} = C_3.$$

Thus,

$$\vec{M}_N = \sum_{i=1}^{3} \vec{M}_{i,N} = (C_1, C_2, C_3) = \vec{M}_0, \qquad N = 1, 2, \dots . \qquad \blacksquare$$

We turn finally to angular momentum. The angular momentum $\vec{L}_{i,n}$ of P_i at t_n is defined to be the vector

$$\vec{L}_{i,n} = m_i(\vec{r}_{i,n} \times \vec{v}_{i,n}).$$

The angular momentum $\vec{L}_n$ of the three-body system at t_n is defined to be

$$\vec{L}_n = \sum_{i=1}^{3} \vec{L}_{i,n}.$$

THEOREM. *Independently of Δt, the numerical method conserves angular momentum, that is,*

$$\vec{L}_n = \vec{L}_0, \qquad n = 1, 2, \dots .$$

PROOF. Note, that

$$\begin{aligned}
\vec{L}_{i,n+1} - \vec{L}_{i,n} &= m_i(\vec{r}_{i,n+1} \times \vec{v}_{i,n+1}) - m_i(\vec{r}_{i,n} \times \vec{v}_{i,n}) \\
&= m_i \left\{ [\vec{r}_{i,n+1} - \vec{r}_{i,n}] \times \left[\frac{\vec{v}_{i,n+1} + \vec{v}_{i,n}}{2}\right] + \left[\frac{\vec{r}_{i,n+1} + \vec{r}_{i,n}}{2}\right] \times [\vec{v}_{i,n+1} - \vec{v}_{i,n}] \right\} \\
&= m_i \left\{ [\vec{r}_{i,n+1} - \vec{r}_{i,n}] \times \left[\frac{\vec{r}_{i,n+1} - \vec{r}_{i,n}}{\Delta t}\right] + \left[\frac{\vec{r}_{i,n+1} + \vec{r}_{i,n}}{2}\right] \times [\vec{v}_{i,n+1} - \vec{v}_{i,n}] \right\} \\
&= \frac{m_i}{2}(\vec{r}_{i,n+1} + \vec{r}_{i,n}) \times (\vec{v}_{i,n+1} - \vec{v}_{i,n}).
\end{aligned}$$

Thus,

$$\vec{L}_{i,n+1} - \vec{L}_{i,n} = \sum_{i=1}^{3} \frac{m_i}{2}(\vec{r}_{i,n+1} + \vec{r}_{i,n}) \times (\vec{v}_{i,n+1} - \vec{v}_{i,n}). \tag{4.3}$$

Substitution of (3.2) into (4.3) and simplification using the laws of cross products yields

$$\vec{L}_{n+1} - \vec{L}_n = \vec{0}, \qquad n = 0, 1, \dots,$$

from which the theorem follows immediately. $\blacksquare$

5. COVARIANCE

Let us turn to covariance next and discuss it as simply as possible. When a dynamical equation is structurally invariant under a transformation, the equation is said to be covariant or symmetric with respect to that transformation. The transformations we will consider are translation, rotation, and uniform relative motion. We will concentrate on

(a) two-dimensional systems,
(b) general Newtonian forces,
(c) motion of a single particle.

This will make the mathematical methodology transparent and will indicate the natural extension to N-body problems in three dimensions.

Suppose then that a particle P of mass m is in motion in the XY plane, and that for $\Delta t > 0$, its motion from given initial data is determined by a force $\vec{F}(t_n) = \vec{F}_n = (F_{x,n}, F_{y,n})$ and the dynamical difference equations

$$\frac{x_{n+1} - x_n}{\Delta t} = \frac{v_{x,n+1} + v_{x,n}}{2}, \qquad \frac{y_{n+1} - y_n}{\Delta t} = \frac{v_{y,n+1} + v_{y,n}}{2}, \tag{5.1}$$

$$F_{x,n} = m\frac{(v_{x,n+1} - v_{x,n})}{\Delta t}, \qquad F_{y,n} = m\frac{(v_{y,n+1} - v_{y,n})}{\Delta t}. \tag{5.2}$$

Our problem is as follows. Let $x = f_1(x^*, y^*)$, $y = f_2(x^*, y^*)$ be a change of coordinates. Under this transformation, let

$$F_{x,n} = F^*_{x^*,n}, F_{y,n} = F^*_{y^*,n}, \qquad \text{and} \tag{5.3}$$

$$\frac{x^*_{n+1} - x^*_n}{\Delta t} = \frac{v^*_{x^*,n+1} + v_{x^*,n}}{2}, \frac{y^*_{n+1} - y^*_n}{\Delta t} = \frac{v_{y^*,n+1} + v_{y^*,n}}{2}. \tag{5.4}$$

We will want to prove that in the X^*Y^* system, the dynamical equations of motion are

$$F^*_{x^*,n} = m\left(\frac{v_{x^*,n+1} - v_{x^*,n}}{\Delta t}\right), \qquad F^*_{y^*,n} = m\left(\frac{v_{y^*,n+1} - v_{y^*,n}}{\Delta t}\right), \tag{5.5}$$

which will establish covariance.

Relative to (5.1) and (5.4), the following lemma will be of value.

LEMMA. *Equations (5.1) and (5.4) imply*

$$v_{x,1} = \frac{2}{\Delta t}(x_1 - x_0) - v_{x,0}, \tag{5.6}$$

$$v_{x^*,1} = \frac{2}{\Delta t}(x^*_1 - x^*_0) - v^*_{x,0}, \tag{5.7}$$

$$v_{x,n} = \frac{2}{\Delta t}\left[x_n + (-1)^n x_0 + 2\sum_{j=1}^{n-1}(-1)^j x_{n-j}\right] + (-1)^n v_{x,0,}, \qquad n \geq 2, \tag{5.8}$$

$$v_{x^*,n} = \frac{2}{\Delta t}\left[x^*_n + (-1)^n x^*_0 + 2\sum_{j=1}^{n-1}(-1)^j x^*_{n-j}\right] + (-1)^n v_{x^*,0,}, \qquad n \geq 2, \tag{5.9}$$

which are also valid if x is replaced by y.

The proof is immediate from (5.1) and (5.4) for $n = 1$ and by mathematical induction for $n > 1$.

THEOREM 5.1. *Equations (5.1) and (5.2) are covariant relative to the translation*

$$x^* = x - a, y^* = y - b.$$

PROOF. Define $v_{x,0} = v_{x^*,0}$, $v_{y,0} = v_{y^*,0}$. Then,

$$\begin{aligned} v_{x,1} &= \frac{2}{\Delta t}(x_1 - x_0) - v_{x,0} = \frac{2}{\Delta t}(x_1^* + a - x_0^* - a) - v_{x^*,0} \\ &= \frac{2}{\Delta t}(x_1^* - x_0^*) - v_{x^*,0} = v_{x^*,1}. \end{aligned}$$

For $n \geq 2$,

$$\begin{aligned} v_{x,n} &= \frac{2}{\Delta t}\left[x_n + (-1)^n x_0 + 2\sum_{j=1}^{n-1}(-1)^j x_{n-j}\right] + (-1)^n v_{x,0} \\ &= \frac{2}{\Delta t}\left[(x_n^* + a) + (-1)^n (x_0^* + a) + 2\sum_{j=1}^{n-1}(-1)^j (x_{n-j}^* + a)\right] + (-1)^n v_{x^*,0} \\ &= v_{x^*,n}, \qquad (n \text{ odd or } n \text{ even}). \end{aligned}$$

Thus, for all n,

$$v_{x,n} = v_{x^*,n}.$$

Similarly,

$$v_{y,n} = v_{y^*,n}.$$

Thus,

$$\begin{aligned} F_{x^*,n}^* &= F_{x,n} = m\frac{v_{x,n+1} - v_{x,n}}{\Delta t} = m\frac{v_{x^*,n+1} - v_{x^*,n}}{\Delta t}, \\ F_{y^*,n}^* &= F_{y,n} = m\frac{v_{y^*,n+1} - v_{y^*,n}}{\Delta t}. \end{aligned}$$

∎

THEOREM 5.2. *Under the rotation*

$$\begin{aligned} x^* &= x\cos\theta + y\sin\theta, \\ y^* &= y\cos\theta - x\sin\theta, \end{aligned}$$

equations (5.1) and (5.2) are covariant.

PROOF. This proof is entirely similar to that of Theorem 5.1.

THEOREM 5.3. *Under relative uniform motion of coordinate systems, equations (5.1) and (5.2) are covariant.*

PROOF. The proof is entirely similar to that of Theorem 5.1, but one utilizes

$$x_n^* = x_n - ct_n, \qquad n = 0, 1, 2, \dots, \qquad \text{and the result}$$

$$t_n + (-1)^n t_0 + 2\sum_{j=1}^{n-1}(-1)^j t_{n-j} = \begin{cases} 0, & n \text{ even}, \\ \Delta t, & n \text{ odd}. \end{cases}$$

6. EXAMPLES

Consider first an utterly simplistic example in which a single particle of unit mass is in motion in a single direction and is acted upon by a constant force. A typical such problem is the classical falling body problem for which $F = -980$ and for which the equations of motion are taken to be

$$\frac{x_{k+1} - x_k}{\Delta t} = \frac{v_{k+1} + v_k}{2}, \tag{6.1}$$

$$\frac{v_{k+1} - v_k}{\Delta t} = -980. \tag{6.2}$$

For (6.1) and (6.2), we can find the particle's position and velocity at any t_n explicitly as follows. Summing both sides of (6.2) from $k = 0$ to $k = n - 1$ implies

$$v_n - v_0 = -980\, n\Delta t,$$

so that

$$v_n = -980\, t_n + v_0. \tag{6.3}$$

Summing both sides of (6.1) from $k = 0$ to $k = n - 1$ and using (6.3) and the fact that the sum of the first n odd integers is n^2 yields

$$\begin{aligned} x_n - x_0 &= \frac{\Delta t}{2} \sum_{k=0}^{n-1} (-980\, t_{k+1} + v_0 - 980\, t_k + v_0) \\ &= \frac{\Delta t}{2} \sum_{k=0}^{n-1} [-980(k+1)\Delta t - 980\, k\Delta t + 2v_0] \\ &= \frac{\Delta t}{2} \left[-980\, n^2 \Delta t + 2v_0 n\right] \\ &= -490\, n^2 (\Delta t)^2 + v_0 n\Delta t, \end{aligned}$$

so that

$$x_n = -490\, t_n^2 - v_0 t_n + x_0. \tag{6.4}$$

Hence, given x_0 and v_0, one can determine x_n and v_n, $n = 1, 2, \ldots$, explicitly by (6.3) and (6.4).

We turn next to a typical application in engineering [4]. Figure 1 shows a particle arrangement for a satellite whose material response is highly nonlinear and elastic. A Saint Venant-Kirchhoff potential is assumed between the particles. Various forces are imposed on the ends A, B, C, D. Figure 2 shows the material response when the dynamical equations are solved in a fully conservative fashion.

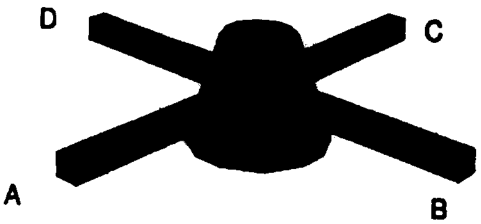


Figure 1.

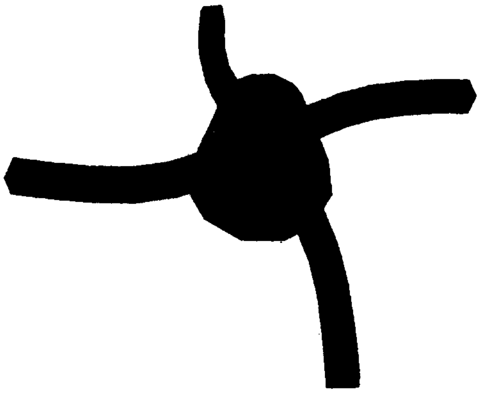


Figure 2.

Next, let us examine the simplest molecule of all, as shown in Figure 3, the ground state H_2 molecule. In this case, we will develop a completely unorthodox, somewhat disturbing model.

The total energy of H_2 is the time invariant $-(50.7289)10^{12}$ erg [5]. The two protons in H_2 vibrate with a characteristic frequency f and with a characteristic bond length d which are given by [5,6]:

$$f = (1.318)10^{14} \text{ cycles/sec } = (1.318)10^{14} H, \tag{6.5}$$

$$d = (0.742)10^{-8} \text{ cm } = (0.742) \text{ Å}. \tag{6.6}$$

Let us see next what happens if we try to simulate the dynamical motions of the two electrons and the two protons in H_2. Use of Newtonian mechanics and coulombic forces is known to be incorrect in the sense that the results do not yield both (6.1) and (6.2). Let us do this, nevertheless, to see how incorrect the results are.

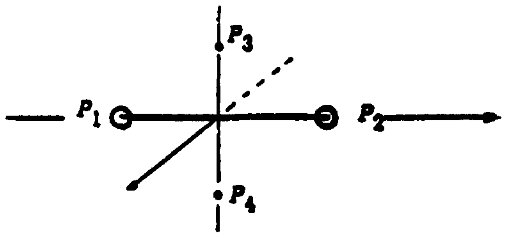


Figure 3.

To test the classical four-body model of H_2 with simple coulombic forces, we applied the method of Section 3 and found that the average diameter was 0.74 Å, which is reasonable, but the average vibrational frequency was $(2.20)10^{14} H$, which is far too excessive. This result supports the use of a quantum mechanics model, rather than a classical Newtonian model. However, in quantum mechanics one often uses shielding; that is, one assumes that the electrons do not feel full coulombic repulsion because of the presence of the protons. So, we chose, instead of full coulombic repulsion between the electrons, only 9/10 of this repulsion. The computed results yielded a correct diameter and a vibrational frequency of $(2.13)10^{14} H$, a modest improvement. We then kept decreasing the factor 9/10 until it was 1/1000, and the resulting diameter was still correct, but the frequency decreased to only $(1.78)10^{14} H$, still incorrect significantly. We then went through 0 and chose the factors $-1/1000$, $-9/10$, -1. For the choice -1, the results were entirely correct. But the choice -1 means that the electrons are attracting rather than repelling. Thus, the model of bonding which results is that bonding electrons attract rather than repel.

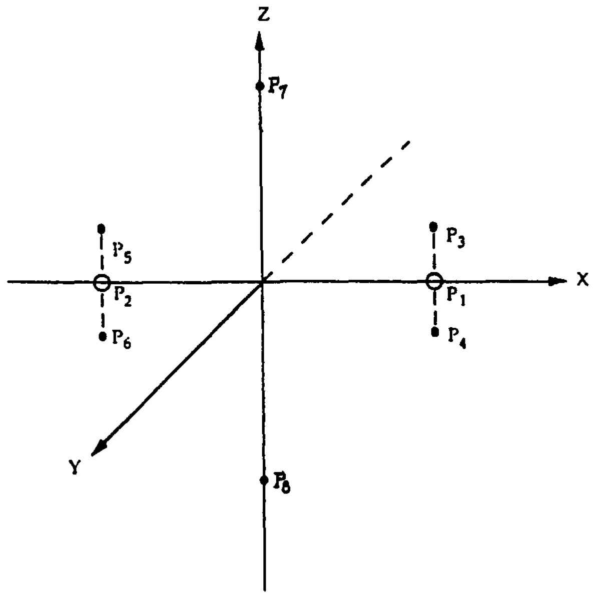
Now, the question arises as to whether electron attraction is possible. First, it should be noted that the quantum mechanical theory of superconductivity is based on the assumption of electron attraction [7]. Second, it should be noted that even though the electron is considered an elementary particle of lepton type, particle physicists are now hypothesizing a subquark structure for electrons, so that electron attraction may be the effect of subquark dynamics [8].

Finally, note that precisely correct results have now been obtained for all isotopic combinations of hydrogen with deuterium and tritium, and for the diatomic molecules Li_2, B_2, C_2, and N_2 [9]. The molecular configurations for these latter four molecules are shown in Figure 4. The choice of attracting electrons is always the pair in furthest separation, so that pairing of electrons also follows in a natural way.

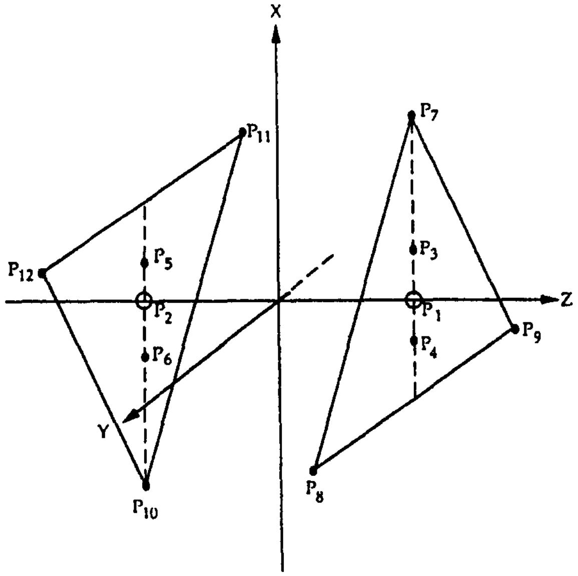
Our results are reminiscent of the famous Einstein quote [10], "You know, it would be sufficient to really understand the electron."

7. REMARKS AND OBSERVATIONS

Difference equation formulations of both special relativity and quantum mechanics have become available recently [2,11]. Nevertheless, if one is interested in dynamics, that is, in how things



(a) Li_2.

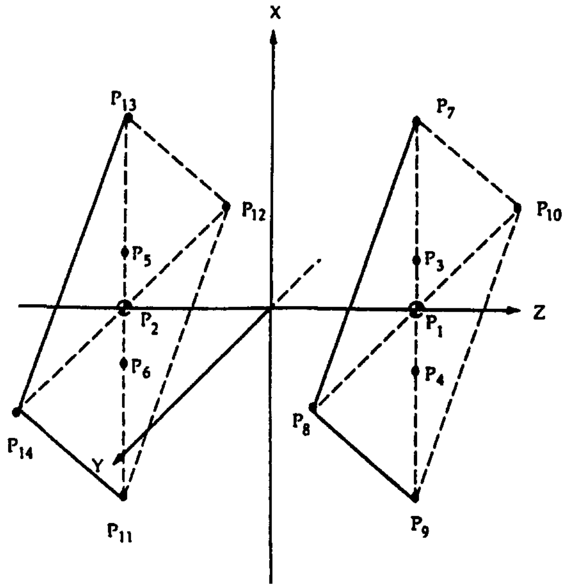


(b) B_2.

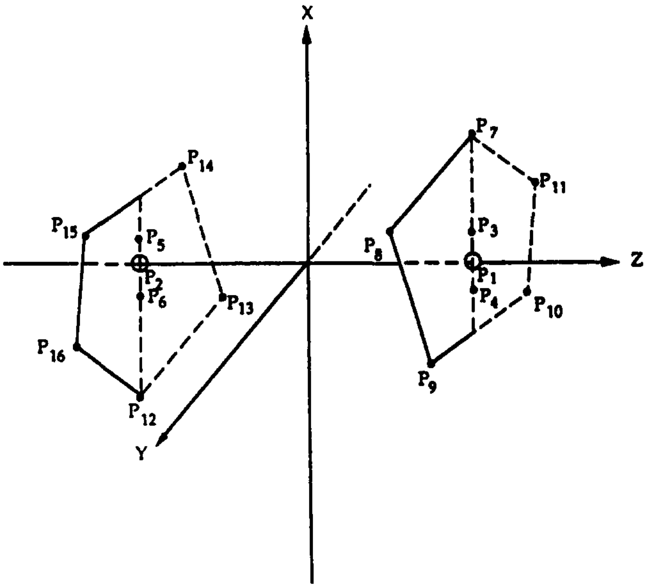
Figure 4.

change with time, then Newtonian physics provides indispensable tools. The reason is that N-body problems for the time dependent Schrödinger equation require $3N+1$ dimensions. Thus, simulation of the solar system by means of quantum mechanics requires 31-dimensional space. On the other hand, relativity denies action-reaction and hence limits N to be 1, so that solar system simulation is not possible at all.

Finally, note that allowing Δt to converge to zero in (2.2), (3.1), (3.2), (6.3), (6.4), and in Theorems 4.1–4.4 yields the formulae and results of classical Newtonian continuum dynamics. However, allowing Δt to converge to zero is a purely mathematical operation which may not be possible physically. Indeed, we are not able to decide whether one can actually construct a clock whose Δt is arbitrarily small, quantum mechanics saying yes, if enough energy is used, and relativity saying no, because of limitations on the speed of light. Thus, on this question, the two modern theories of physics are in disagreement.



(c) C_2.



(d) N_2.

Figure 4. (cont.)

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